

A note on random walks in a hypercube

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Abstract

We study a simple random walk on an n -dimensional hypercube. For any starting position we find the probability of hitting vertex a before hitting vertex b , whenever a and b share the same edge. This generalizes the model in [2] (see Exercise 1.3.7 there).

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Consider an n -dimensional hypercube, that is a graph with 2^n vertices in the set $\{0, 1\}^n$. A vertex x of a hypercube can be encoded by a sequence $x = (x_1, x_2, \dots, x_n)$ where each x_i is either 0 or 1.

Two vertices $x = (x_1, x_2, \dots, x_n)$ and $y = (y_1, y_2, \dots, y_n)$ are connected by an edge, if and only if $\sum_{i=1}^n |x_i - y_i| = 1$, that is x and y differ in exactly one coordinate (for example when $n = 5$, $x = (0, 1, 0, 1, 0)$, and $y = (0, 0, 0, 1, 0)$). For two vertices x and y the (graph) distance between them is the quantity $|x - y| := \sum_{i=1}^n |x_i - y_i|$, that is the smallest number of edges on the path connecting x and y .

A simple random walk on a hypercube is a particle which moves from one vertex to another along the edges of this graph, with equal probabilities.

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Since each vertex is connected by an edge to exactly n other vertices, the probability to go to any particular neighbor equals $1/n$, and is independent of the past movements. Such a walk has been fairly extensively studied, especially its asymptotic properties, but we were not able to find in the published materials the exact formula found by us in Theorem 1. Probably the most relevant references for the walk on the hypercube would be [1], [2] and [3], which of course does not expire the set of the available literature on the topic.

Suppose we have two distinct vertices a and b . Start a random walk at some point $X_0 = x$ and denote its position at time n as X_n . Assume that the walk stops when it hits either a or b . Our aim is to compute the probability that X_n hits b before it hits a . Formally, if

$$\tau = \inf\{n \geq 0 : X_n = a \text{ or } b\}$$

we want to compute

$$p_{a,b}(x) = \mathbb{P}(X_\tau = b \mid X_0 = x).$$

Though we were not able to answer this question in general, we can do it nonetheless in the case when a and b are immediate neighbors, that is, connected by an edge. Without loss of generality, assume from now on that

$$a = (0, 0, \dots, 0, 0)$$

and

$$b = (0, 0, \dots, 0, 1).$$

See Figure 1 for a possible location of point x .

Theorem 1 *Suppose we start a simple random walk on the hypercube from point $x = (x_1, x_2, \dots, x_n)$. Then the probability that this walk hits b before a ,*

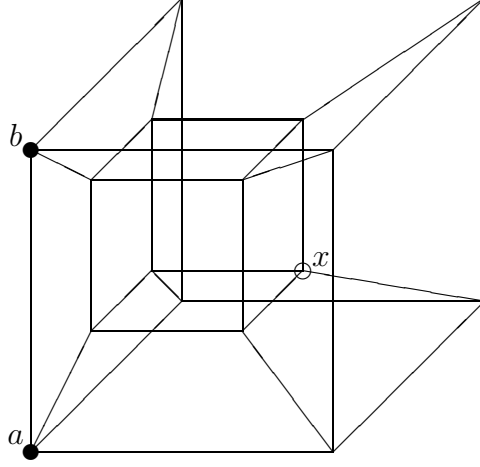


Figure 1: A 4-dimensional hypercube. $a = (0, 0, 0, 0)$, $b = (0, 0, 0, 1)$ and $x = (1, 1, 1, 0)$.

is

$$p(x) = p_{a,b}(x) = \begin{cases} \frac{1}{2} - \frac{\sum_{i=k+1}^n \binom{n}{i}}{2(2^n - 1) \binom{n-1}{k}}, & \text{if } x_n = 0; \\ \frac{1}{2} + \frac{\sum_{i=k+1}^n \binom{n}{i}}{2(2^n - 1) \binom{n-1}{k}}, & \text{if } x_n = 1, \end{cases}$$

where $k = x_1 + x_2 + \cdots + x_{n-1}$.

PROOF: As it is noted in [2], instead of finding the probability $p(x)$ we can solve a seemingly completely different problem from electric networks as follows. Suppose that each edge of the hypercube is replaced by a unit resistor. Attach a 1 volt battery to points a and b , such that the voltage at a , denoted as $v(a)$, equals 0, and the voltage at b is $v(b) = 1$. Then the voltage

at vertex x , denoted by $v(x)$ is equal exactly to the unknown probability $p(x)$.

Thus, to solve our problem, we will use the language and the methods borrowed from electric network theory. For example, if two or more resistors are connected in series, they may be replaced by a single resistor whose resistance is the sum of their resistances. Also, m (≥ 2) resistors in parallel may be replaced by a single resistor with resistance R equal to $1/(R_1^{-1} + \dots + R_m^{-1})$ where R_1, \dots, R_m are the resistances of the original resistors.

From the symmetry it follows that the voltage at all vertices of the cube lying in the set

$$W_k := \{x = (x_1, x_2, \dots, x_{n-1}, 0) \text{ such that } x_1 + x_2 + \dots + x_{n-1} = k\}$$

is the same and depends on k only. Let us denote this voltage w_k . Similarly, the voltage at all vertices in

$$W_k := \{x = (x_1, x_2, \dots, x_{n-1}, 1) \text{ such that } x_1 + x_2 + \dots + x_{n-1} = k\}$$

is also the same, let us denote this voltage \tilde{w}_k . Moreover, from symmetry, the probability to hit $a = (0, \dots, 0, 0)$ before $b = (0, \dots, 0, 1)$ starting from $(x_1, x_2, \dots, x_{n-1}, 0)$ is the same as the probability to hit b before a starting from $(x_1, x_2, \dots, x_{n-1}, 1)$, we obtain

$$\tilde{w}_k = 1 - w_k, \text{ for } k = 0, 1, \dots, n-1. \quad (1)$$

Obviously, we have

$$w_0 = 0. \quad (2)$$

Now for $1 \leq k \leq n-1$, the vertex $x = (x_1, x_2, \dots, x_{n-1}, 0) \in W_k$ is connected

to n vertices

$$\begin{aligned}
& (1 - x_1, x_2, \dots, x_{n-1}, 0) \\
& (x_1, 1 - x_2, \dots, x_{n-1}, 0) \\
& \dots \\
& (x_1, x_2, \dots, 1 - x_{n-1}, 0) \\
& (x_1, x_2, \dots, x_{n-1}, 1)
\end{aligned}$$

where the last one lies in \tilde{W}_k , and among the first $n-1$ vertices k lie in W_{k-1} and $n-1-k$ in W_{k+1} (since there are exactly k ones and $n-1-k$ zeros in the set $\{x_1, x_2, \dots, x_{n-1}\}$). From Kirchhoff's and Ohm's Laws, stating that the sum of all currents from a vertex is zero, and the current that flows through an edge equals the difference in voltages divided by the resistance of that edge (which are all one in our case), we conclude that

$$k \times \frac{w_{k-1} - w_k}{1} + (n-1-k) \times \frac{w_{k+1} - w_k}{1} + \frac{\tilde{w}_k - w_k}{1} = 0$$

whence taking into account (1)

$$w_k = \frac{k w_{k-1} + (n-k-1) w_{k+1} + 1}{n+1}, \quad k = 1, 2, \dots, n-2. \quad (3)$$

Additionally, for $k = n-1$, we obtain in the same way

$$w_{n-1} = \frac{(n-1) w_{n-2} + 1}{n+1}. \quad (4)$$

Thus we have to solve the system of equations (2), (3), and (4). To this end, first set $w_k = \frac{1}{2} - u_k$ for all k , then our system becomes

$$\begin{aligned}
u_0 &= 1/2, \\
u_k &= \frac{k u_{k-1} + (n-k-1) u_{k+1}}{n+1}, \quad k = 1, 2, \dots, n-1,
\end{aligned} \quad (5)$$

with the additional condition $u_n = 0$ (its value does not matter anyway since it is multiplied by 0 for $k = n-1$). Note that intuitively we must end up

with $u_k \geq 0$, since every vertex $x \in W_k$ is closer to a than to b . Thus the probability w_k to hit b before a should not exceed $\frac{1}{2}$.

We can rewrite system (5) as

$$\begin{aligned} u_0 &= 1/2, \\ u_{k-1} &= \frac{(n+1)u_k - (n-k-1)u_{k+1}}{k}, \quad k = 1, 2, \dots, n-1. \end{aligned} \tag{6}$$

Solving system (6) backwards, we obtain

$$\begin{aligned} u_{n-2} &= \frac{n+1}{n-1}u_{n-1}, \\ u_{n-3} &= \frac{n^2+n+2}{(n-1)(n-2)}u_{n-1} \\ u_{n-4} &= \frac{n^3+5n+6}{(n-1)(n-2)(n-3)}u_{n-1} \end{aligned}$$

etc. With some guessing, one can notice that

$$iu_{i-1} = nu_{n-1} + (n-i)u_i \tag{7}$$

for $i = n, n-1, n-2, n-3$. Let us prove by induction that this is true for all $i = 1, \dots, n$. Indeed, we already know that (7) holds for $i = n, \dots, n-3$. Suppose that (7) holds for $i = k+1, k+2, \dots, n$. Let us establish (7) for $i = k$. Indeed, from (6), plugging in (7) with $i = k+1$, we obtain

$$u_{k-1} = \frac{(n+1)u_k - (n-k-1)u_{k+1}}{k} = \frac{(n+1)u_k - [(k+1)u_k - nu_{n-1}]}{k}$$

yielding $ku_{k-1} = nu_{n-1} + (n-k)u_k$ and thus completing the induction.

In the next step we want to compute u_i as a function of u_{n-1} . Let us denote $u_{n-1} = c$ and substitute

$$z_i = (i+1)(i+2) \dots (n-1)u_i$$

into (7). Then we have $z_{n-2} = (n+1)c$ and

$$z_{i-1} = n(n-1) \dots (i+1)c + (n-i)z_i$$

which after reiterations gives

$$\begin{aligned}
z_{n-j-1}/c &= n(n-1)\dots(n-j+1) \times 1 \\
&+ n(n-1)\dots(n-j+2) \times j \\
&+ n(n-1)\dots(n-j+3) \times j(j-1) \\
&+ \dots \\
&+ n(n-1) \times j(j-1)\dots 3 \\
&+ n \times j(j-1)\dots 3 \cdot 2 \\
&+ 1 \times j(j-1)\dots 3 \cdot 2 \cdot 1,
\end{aligned}$$

that is,

$$z_{n-j-1} = c \sum_{l=0}^j \frac{n!}{(n-j+l)!} \frac{j!}{(j-l)!} = cj! \sum_{l=0}^j \binom{n}{j-l}.$$

Recalling that $u_0 = 1/2$ gives $z_0 = (n-1)!/2$ whence

$$\begin{aligned}
\frac{(n-1)!}{2} &= z_0 = c(n-1)! \sum_{l=0}^{n-1} \binom{n}{n-1-l} = c(n-1)! \sum_{l=0}^{n-1} \binom{n}{l+1} \\
&= c(n-1)! \sum_{l=1}^n \binom{n}{l} = c(n-1)! (2^n - 1).
\end{aligned}$$

Therefore, $c = 1/(2^{n+1} - 2)$,

$$z_k = \frac{(n-1-k)! \sum_{l=0}^{n-1-k} \binom{n}{n-1-k-l}}{2^{n+1} - 2}$$

and

$$u_k = \frac{k!}{(n-1)!} z_k = \frac{\sum_{l=0}^{n-1-k} \binom{n}{n-1-k-l}}{\binom{n-1}{k} (2^{n+1} - 2)} = \frac{\sum_{i=k+1}^n \binom{n}{i}}{\binom{n-1}{k} (2^{n+1} - 2)},$$

Recalling that $w_k = 1/2 - u_k$ and hence $\tilde{w}_k = 1/2 + u_k$ finishes the proof.

QED

Remark 1 If $a = (0, 0, \dots, 0)$ and $b = (1, 1, \dots, 1)$, so that the points a and b are the furthestmost points of the hypercube, one can compute $p_{a,b}(x)$ very

easily (we leave this as an exercise). However, with the exception of the two cases when $|a - b| = 1$ and $|a - b| = n$ we do not know a general formula for $p_{a,b}(x)$.

Remark 2 On the other hand, the formula for the probability that the walk started at $a = (0, 0, \dots, 0)$ is located at vertex $x = (x_1, x_2, \dots, x_n)$ at time N with $|x| = \sum_{i=1}^n x_i = k$ is known and given by formula (3.1) in [1]:

$$\frac{1}{2^n} \sum_{j=0}^n n \left[1 - \frac{2j}{n+1} \right]^N \sum_{i=0}^k (-1)^i \binom{k}{i} \binom{n-k}{j-i}.$$

References

- [1] DIACONIS P., MORRISON J.A., and GRAHAM, R.L., *Asymptotic Analysis of a Random Walk on a Hypercube with Many Dimensions*, Random Structures Algorithms, Vol. 1, pp. 51-72, 1990.
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- [3] VOIT M., *Ehrenfest urn and related random walks*, J. Appl. Probab., Vol. 33, pp. 340-356, 1996.